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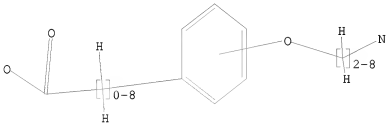


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Structure attributes must be viewed using STN Express query preparation.


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   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 11:01:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  2514382 TO ITERATE

 38.0% PROCESSED   956360 ITERATIONS                              1018 ANSWERS

 39.8% PROCESSED  1000000 ITERATIONS                              1060 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.24

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      2514382 TO  2514382
PROJECTED ANSWERS:            2511 TO     2819

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L3          135 L2

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L4            9 L3 AND PY<2002
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L4 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:208799 CAPLUS
DOCUMENT NUMBER: 148:275678
TITLE: Vitronectin receptor antagonist pharmaceuticals
INVENTOR(S): Rajopadhye, Milind; Barrett, John A.; Carpenter, Jr., Alan P.; Cheesman, Edward H.; Harris, Thomas D.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA
SOURCE: U.S., 133pp., Cont.-in-part of U.S. Ser. No. 466,588. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
US 7332149	B1	20080219	US 2000-599890	20000621	
US 6322770	B1	20011127	US 1999-281207	19990330	<--
US 20020015680	A1	20020207	US 1999-281209	19990330	
US 6524553	B2	20030225			
US 6548663	B1	20030415	US 1999-281050	19990330	
US 6794518	B1	20040921	US 1999-466588	19991217	
US 20030124120	A1	20030703	US 2002-269252	20021011	
US 20030149262	A1	20030807	US 2002-306054	20021126	
US 20050154185	A1	20050714	US 2004-770380	20040202	
US 7321045	B2	20080122			

PRIORITY APPLN. INFO.:

US 1998-112829P	P	19981218
US 1999-466588	A2	19991217
US 1998-80150P	P	19980331
US 1998-112715P	P	19981218
US 1998-112732P	P	19981218
US 1998-112831P	P	19981218
US 1999-281050	A3	19990330
US 1999-281209	A3	19990330

GI

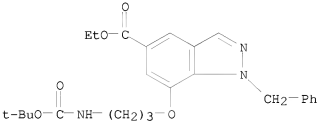
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention describes novel compds. comprising at least one of a chemotherapeutic agent or a radiosensitizer agent, and further comprising a diagnostic or therapeutic metallopharmaceutical selected from defined 99mTc complexes, e.g., 99mTc(L)(tricine)(TPPTS) where L = diazenido derivative of polyfunctional benzenesulfonic acid I and TPPTS = tris(m-sulfophenyl)phosphine trisodium salt, or various indium, lutetium, yttrium or gadolinium polyfunctionalized DOTA-type complexes, e.g., indium complex II, useful for the diagnosis and treatment of cancer, methods of imaging tumors in a patient, and methods of treating cancer in a patient. The pharmaceuticals are thus comprised of a targeting moiety that binds to the vitronectin receptor that is expressed in tumor vasculature, an optional linking group, and a therapeutically effective radioisotope or

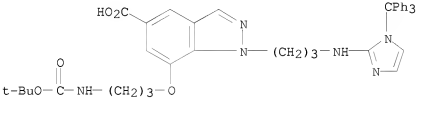
diagnostically effective imageable moiety. The present invention also provides novel compds. useful for monitoring therapeutic angiogenesis treatment and destruction of new angiogenic vasculature. The present invention also provides novel compds. useful for imaging atherosclerosis, restenosis, cardiac ischemia, and myocardial reperfusion injury. The present invention also provides novel compds. useful for the treatment of rheumatoid arthritis. The pharmaceuticals are comprised of a targeting moiety that binds to a receptor that is upregulated during angiogenesis, an optional linking group, and a therapeutically effective radioisotope or diagnostically effective imageable moiety. The imageable moiety is a gamma ray or positron emitting radioisotope, a magnetic resonance imaging contrast agent, an x-ray contrast agent, or an ultrasound contrast agent.

IT 1007219-80-8P 1007219-81-9P
RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(vitronectin receptor antagonist metallopharmaceuticals as chemotherapeutic or radiosensitizer agents)

RN 1007219-80-8 CAPLUS
CN 1H-Indazole-5-carboxylic acid, 7-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propoxy]-1-(phenylmethyl)-, ethyl ester (CA INDEX NAME)



RN 1007219-81-9 CAPLUS
CN 1H-Indazole-5-carboxylic acid, 7-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propoxy]-1-[3-[[1-(triphenylmethyl)-1H-imidazol-2-yl]amino]propyl]- (CA INDEX NAME)



REFERENCE COUNT: 148 THERE ARE 148 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:20052 CAPLUS
DOCUMENT NUMBER: 64:20052

ORIGINAL REFERENCE NO.: 64:3741b-g
TITLE: Aminoarylideneacetonitrile dyes
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: 16 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6500517		19650719	NL 1965-517	19650115 <--
BE 658426			BE	
FR 1425609			FR	

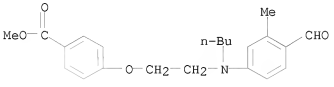
PRIORITY APPLN. INFO.: DE 19640117
GI For diagram(s), see printed CA Issue.
AB Greenish yellow dyes of the general formula I for polyester fabrics were prepared; in formula I, R is H or Me, R1 Et, Bu, or PhOCH2CH2, R2 = H or MeO2C, X = CN or CO2Et, and Y is CO2, OCO2, or O. Bu(HOCH2CH2)NPh (II) 19.3, C6H6 100, powdered K2CO3 13.8, present with p-MeO2CC6H4COCl 19.9 parts, and the product 35.5 parts, b0.6 230-5°, in 100 parts PhCl added dropwise at 50-5° to 30.7 parts POCl3 and 14.6 parts HCONMe2 and stirred 12 hrs. at 50-5° yielded p-MeO2CC6H4CO2CH2CH2N(Br)C6H4CHO-p (III). III 38, NCCH2CO2Et 12, EtOH 20, and piperidine 1 part refluxed 2 hrs. yielded yellow I (R = H, R1 = Bu, R2 = p-MeO2C, X = CO2Et, Y = CO2), m. 120-1° (EtOH); it dyes polyester, polyamide, and triacetylcellulose fabrics greenish yellow shades of very good fastness properties. III with CH2(CN)2 gave similarly I (R = H, R1 = Bu, R2 = p-MeO2C, X = CN, Y = CO2), m. 88-90°. II (20.7 parts) treated with 19.9 parts p-MeO2CC6H4COCl and 11 parts Et3N at 80-100°, and the condensation product formylated yielded 2,4-Me[p-MeO2CC6H4CO2CH2CH2N(Bu)]C6H3CHO; a 40-part portion in 100 cc. Et3N with 7 parts CH2(CN)2 in BuOH yielded greenish yellow I (R = Me, R1 = Bu, R2 = MeO2C, X = CN, Y = CO2), m. 112-14° (EtOH). Et(HOCH2CH2)NPh condensed with o-MeO2CC6H4COCl and then formylated, and the resulting 2,4-Me[o-MeO2CC6H4CO2CH2CH2N(Et)]C6H3CHO treated with CH2(CN)2 yielded I (R = Me, R1 = Et, R2 = o-MeO2C, X = CN, Y = CO2), m. 100-1°. 3-Me derivative of II condensed with p-ClCO2C6H4CO2Me, and the product heated to 150-200°, distilled (b0.5-0.6 198-207°), and then formylated with POCl3-HCONMe2 gave 2,4-Me[p-MeO2CC6H4OCH2CH2N(Bu)]C6H3CHO, b1.6 279-80°, which with CH2(CN)2 yielded I (R = Me, R1 = Bu, R2 = p-MeO2C, X = CN, Y = O), m. 84-7°. m-MeC6H4N(CH2CH2Cl)Et (IV) 59.5, HCONMe2 100, and PhONa 34.8 parts gave m-McC6H4N(CH2CH2OPh)Et, b0.8 155-63°, which formylated and condensed with NCCH2CO2Et yielded I (R = Me, R1 = Et, R2 = H, X = CO2Et, Y = O), m. 74-5°. IV 59.8, HCONMe2 357, and p-MeO2CC6H4CO2K 72.5 parts heated 7 hrs. at 140°, concentrated, and treated with 95 parts POCl3 yielded 2,4-Me[p-MeO2CC6H4CO2CH2CH2N(Et)]C6H3CHO, m. 77-80°, which condensed with CH2(CN)2 yielded I (R = Me, R1 = Et, R2 = p-EtO2C, X = CN, Y = CO2), m. 136-8°. m-MeC6H2N(CH2CH2OH)Et 71.5 with ClCO2Ph 69.0 and Et3N 44.5 parts gave m-MeC6H3N(CH2CH2OCO2Ph)Et which formylated and condensed with CH2(CN)2 yielded I (R = Me, R1 = Et, R2 = H, X = CN, Y = OCO2). m-MeC6H4(CH2CH2Cl)2 23.2, NaOPh 24, and (MeOCH2CH2)2O 50 parts refluxed 1-2 hrs., and the product formylated gave 2,4-Me[(PhOCH2CH2)2N]C6H3CHO, m. 82-4° (EtOH), which condensed with

CH2(CN)2 yielded I (R = Me, R1 = PhOCH2CH2, R2 = H, X = CN, Y = O); it dyes greenish yellow shades.

IT 1081794-87-7P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Aminoarylideneacetonitrile dyes)

RN 1081794-87-7 CAPLUS

CN Benzoic acid, 4-[2-[butyl(4-formyl-3-methylphenyl)amino]ethoxy]-, methyl ester (CA INDEX NAME)



L4 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:408695 CAPLUS
DOCUMENT NUMBER: 59:8695
ORIGINAL REFERENCE NO.: 59:1531d-h,1532a-d
TITLE: Quaternary ammonium salts from tertiary 2-phenoxyethylamines
INVENTOR(S): Copp, Frederick C.; Elphick, Albert R.; Coker, Geoffrey G.
PATENT ASSIGNEE(S): Wellcome Foundation Ltd.
SOURCE: 13 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 919126		19630220	GB	19580701 <--
PRIORITY APPLN. INFO.:			GB	19580701

GI For diagram(s), see printed CA Issue.

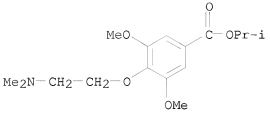
AB (Phenoxyalkyl)dialkylamines are treated with alkyl halides to give I and II, where R and R1 are Me or Et, R2 and R3 are H, halogen, MeO, or Me, Y is NO2, Cl, an alkyl, or an alkoxy group, Z is a C1-3 alkoxy group, and X is iodine or Br; I and II can be used as depressants for the peripheral sympathetic nervous system. Thus, 136 g. 4-hydroxy-3,5-dimethylbenzophenone is added to a solution of 13.8 g. Na in 950 mL. hot EtOH, 136 g. BrCH2CH2Br added, the mixture refluxed 7 h., .apprx.700 mL. EtOH evaporated in vacuo, the residue poured into 500 mL. H2O, the oil that sep. extracted with Et2O, the extract washed with 5N NaOH, the Et2O evaporated, and the residue distilled to give 2-(4-benzoyl-2,6-dimethylphenoxy)ethyl bromide (III), b0.01 182-6°, m.p. 76°. A mixture of 16.7 g. III and 50 g. 25% Me2NH(MeOH) is heated in a sealed tube at 100° 6 h., the mixture evaporated, excess 5N NaOH added to the residue, the oil that sep. extracted with Et2O, the Et2O evaporated, and the residue distilled to give 1-(4-benzoyl-2,6-dimethylphenoxy)-2-dimethylaminoethane (IV), b0.001

162-7°. MeI (4 g.) is added to a solution of 4 g. IV in Me2CO, the mixture kept 1 h., refluxed 30 min., and cooled to give N-[2-(4-benzoyl-2,6-dimethylphenoxy)ethyl]-N,N,N-trimethylammonium iodide, m. 208-9° (EtOH). Similarly prepared are I (Y, R2, R3, R, R1, X, m.p. given): H, Me, Me, Me, Et, iodine, 185-6° (EtOH); H, Me, Me, Me, Me, Br, 204-5° (iso-PrOH); p-Me, Me, Me, Me, Me, Br (hemihydrate), 216-17° (EtOH-iso-PrOH); m-Me, Me, Me, Me, Me, Br, 221°; o-Cl, Me, Me, Me, Me, Br, 204-5°; m-Cl, Me, Me, Me, Me, Br, 203-4°; p-Cl, Me, Me, Me, Me, Br, 226-7°; o-MeO, Me, Me, Me, Me, Br, 216-17°; m-MeO, Me, Me, Me, Me, Br, 176-8°; p-MeO, Me, Me, Me, Me, Br, 189-90°; p-EtO, Me, Me, Me, Me, Br, 203°; p-NO2: Me, Me, Me, Me, Br, 240-1°; H, Cl, Cl, Me, Me, Br, 186°, H, H, H, Me, Me, Br, 196-7°; p-NH2, Me, Me, Me, Me, iodine, 239-41°; H, H, Br, Me, Me, iodine, 209-10° (MeOH); H, H, Br, Me, Et, iodine, 165-6°; H, H, Cl, Me, Me, Br, 199-200° (iso-PrOH-Et2O); H, H, F, Me, Me, iodine, 227-80°; H, H, F, Me, Et, iodine (hemihydrate), 211-12°; H, Br, Me, Me, Me, iodine, 178-9° (EtOH-iso-PrOH); H, Me, Et, Me, Et, iodine, 221-2°; H, Me, Me, Me, HO(CH2)2, iodine, 160-1° (EtOH); H, Me, Me, HO(CH2)2, HO(CH2)2, iodine, 110-11°; H, Me, Me, Et, Et, iodine, 149-50° (EtOH); H, H, MeO, Me, Me, iodine, 189-90° (EtOH-ether); H, Me, Me, Me, Me, Cl (hydrate), 209° (iso-PrOH-Et2O); and H, Me, Me, Me, Me, MeSO4, 138-9° (EtOH-EtOAc). Similarly prepared are II (Z, R2, R3, R, R1, X, m.p. given): Me, Me, Me, Me, Me, iodine, 182-3° (EtOH); Et, Me, Me, Me, Me, iodine, 181-2° (EtOH); Et, Me, Me, Me, Et, Br, 109-11° (iso-PrOH-Et2O); PhCH2, Me, Me, Me, Me, Br, 148-50° (iso-PrOH); EtO, H, H, Me, Me, iodine, 157-60° (EtOAc-EtOH); MeO, H, H, Me, Me, iodine, 205-7° (Me2CO-EtOAc); MeO, Me, H, Me, Me, iodine, 149-51° (EtOH-EtOAc); MeO, Me, Me, Me, Me, iodine, 213-15° (EtOH-EtOAc); EtO, H, H, Et, Et, iodine, 128° (EtOH-EtOAc); EtO, Me, H, Me, Me, iodine, 163-5° (EtOH-EtOAc); iso-PrO, Me, Me, Me, Me, iodine, 186-7° (iso-PrOH); MeO, MeO, H, Me, Me, iodine 181-4° (EtOH); EtO, MeO, H, Me, Me, iodine, 136-8° (EtOH); EtO, MeO, MeO, Me, Me, iodine, 208-10° (EtOH); MeO, Br, H, Me, Me, iodine, 196-9° (EtOH); MeO, Br, H, Me, Et, iodine, 186-9° (EtOH); EtO, Br, H, Me, Me, iodine, 184-5° (iso-PrOH); EtO, Br, H, Me, Et, iodine, 121-4° (iso-PrOH); and EtO, Me, Me, Me, Me, iodine, 177-9° (EtOH-EtOAc). Also prepared are (m.p. given) N-[3-(4-benzoyl-2,6-dimethylphenoxy)propyl]-N,N,N-trimethylammonium bromide, 160-1°; N-[2-(4-benzoyl-2,6-dimethylphenoxy)-1-methylethyl]-N,N,N-trimethylammonium iodide, 215-16° (EtOH); N-[2-(4-benzoyl-2,6-dimethylphenoxy)-2-methylethyl]-N,N,N-trimethylammonium iodide, 167° (EtOH); N-[2-(4-benzoyl-3-hydroxyphenoxy)ethyl]-N,N,N-trimethylammonium iodide, 139-40° (EtOH); N-[2-(4-acetamido-2,6-dimethylphenoxy)ethyl]-N,N,N-trimethylammonium iodide, 242-4° (MeOH); and N-[2-(4-propionylamino-2,6-dimethylphenoxy)ethyl]-N,N,N-trimethylammonium iodide, 197-9° (EtOH).

IT 875831-55-3P, Benzoic acid, 4-[2-(dimethylamino)ethoxy]-3,5-dimethoxy-, isopropyl ester
RL: PREP (Preparation)
(preparation of)

RN 875831-55-3 CAPLUS

CN Benzoic acid, 4-[2-(dimethylamino)ethoxy]-3,5-dimethoxy-, 1-methylethyl ester (CA INDEX NAME)



L4 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:408694 CAPLUS
DOCUMENT NUMBER: 59:8694
ORIGINAL REFERENCE NO.: 59:1531c-d
TITLE: Catalytic reduction of haloaromatic nitro compounds to haloaromatic amines
INVENTOR(S): Dietzler, Andrew J.; Keil, Theodore R.
PATENT ASSIGNEE(S): Dow Chemical Co.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

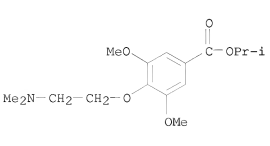
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3067253		19621204	US 1958-746334	19580703 <--
PRIORITY APPLN. INFO.:			US	19580703

AB Good yields of haloaromatic amines are obtained from the catalytic hydrogenation of haloaromatic nitro compds. in the presence of 0.1-0.3 g. Ca(OH)2 per g. Raney Ni catalyst. Thus, the following redns. were carried out: m-BrC6H4NO2 to m-BrC6H4NH2, 83-7%; 4,3-Br(O2N)C6H3Ph to 4,3-Br(H2N)C6H3Ph, 86.3%; 3,4-Br(O2N)C6H3OH to 3,4-Br(H2N)C6H3OH, 72.9%; 3,4-Cl2C6H3NO2 to 3,4-Cl2C6H3NH2, 91.3%; and 2,5-Br2C6H3NO2 to 2,5-Br2C6H3NH2, 88.5%. CaCO3, Ca(OAc)2, Mg(OH)2, NaOAc, or Na2CO3 may be used in place of Ca(OH)2.

IT 875831-55-3P, Benzoic acid, 4-[2-(dimethylamino)ethoxy]-3,5-dimethoxy-, isopropyl ester
RL: PREP (Preparation)
(preparation of)

RN 875831-55-3 CAPLUS

CN Benzoic acid, 4-[2-(dimethylamino)ethoxy]-3,5-dimethoxy-, 1-methylethyl ester (CA INDEX NAME)



L4 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1954:28918 CAPLUS
DOCUMENT NUMBER: 48:28918
ORIGINAL REFERENCE NO.: 48:5219h-i,5220a-c
TITLE: Quaternary ammonium salts of tertiary aminoalkyl 2-(tertiary aminoalkoxy)-4-substituted-benzoates
INVENTOR(S): Clinton, Raymond O.; Laskowski, Stanley C.
PATENT ASSIGNEE(S): Sterling Drug Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

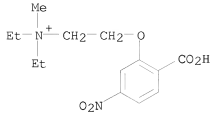
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2642435		19530616	US 1951-245249	19510905 <--

AB Preparation and properties are described for series of compds. having 2 quaternary ammonium groups, which have ganglionic blocking activity. Thus, 2-(tertiaryaminoalkoxy)-4-nitrobenzoic acids are heated in refluxing EtOH or PrOH with a tertiary-aminoalkyl halide to yield tertiary aminoalkyl 2-(tertiary aminoalkoxy)-4-nitrobenzoates. These are reacted with 2 equivalent of MeI to form the corresponding dibasic quaternary ammonium salts. The nitro groups are then reduced by catalytic hydrogenation. Thus, 15.9 g. of 2-(2-diethylaminoethoxy)-4-nitrobenzoic acid-HCl, 8.1 g. Et2NCH2CH2Cl, and 200 ml. iso-PrOH are refluxed 7 hrs. and allowed to stand overnight. Purification yielded a straw-colored oil, 2-diethylaminoethyl 2-(2-diethylaminoethoxy)-4-nitrobenzoate (I) (di-HCl salt, m. 193-3.9°). To a solution of 4.8 g. of I in 125 ml. of EtOAc was added 20 ml. of MeI at room temperature After standing overnight, precipitate was removed, washed, and recrystd. from absolute alc. to yield the dimethiodide (II) of I. II was reduced with H under reduced pressure at 50° in absolute alc. to give 2-diethylaminoethyl 2-(2-diethylaminoethoxy)-4-aminobenzoate-MeI, m. 210.5-11.9°. Similar preparation is described for 3-piperidinopropyl 2-(2-diethylaminoethoxy)-4-nitrobenzoate-2HCl, m. 214.4-15.2°; 2-morpholinoethyl 2-(2-diethylaminoethoxy)-4-nitrobenzoate-2HCl, m. 217-18°; 3-piperidinopropyl 2-(3-piperidinolpropoxy)-4-nitrobenzoate-2HCl, m. 213-14.1 (di-MeI, m. 203.6-4.2); 3-piperidinopropyl 2-(2-diethylaminoethoxy)-4-nitrobenzoate-2MeI, m. 113.4-15.5; 2-(2-methylpiperidinoethyl 2-(2-diethylaminoethoxy)-4-nitrobenzoate-2MeI, m. 201.1-2.9. All m.ps. are corrected Cf. preceding abstract

IT 878796-24-8, Ammonium, [2-(2-carboxy-5-nitrophenoxy)ethyl]diethylmethyl-, iodide (esters)

RN 878796-24-8 CAPLUS

CN Ethanaminium, 2-(2-carboxy-5-nitrophenoxy)-N,N-diethyl-N-methyl-, iodide (1:1) (CA INDEX NAME)



● I⁻

L4 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1954:28917 CAPLUS
DOCUMENT NUMBER: 48:28917
ORIGINAL REFERENCE NO.: 48:5219b-h
TITLE: Quaternary ammonium salts of lower alkyl 2-(tertiary aminoalkoxy)-4-substituted-benzoates
INVENTOR(S): Clinton, Raymond O.; Laskowski, Stanley C.
PATENT ASSIGNEE(S): Sterling Drug Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2642434		19530616	US 1951-245248	19510905 <--

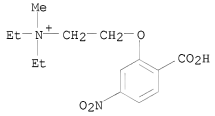
AB The preparation of a series of quaternary ammonium compds. having ganglionic-blocking activity (cf. C.A. 46, 6108e; 44, 6403b) is described. Thus, to 42.2 g. 4,2-O2N(HO)C6H3CO2Et in 1 l. refluxing absolute alc. was added 4.6 g. Na in 500 ml. absolute alc., then 27.1 g. Et2NCH2CH2Cl (I). 5 g. more I added after 3 hrs., refluxing continued 0.5 hr., the mixture cooled in ice, filtered, the filtrate evaporated to dryness in vacuo, the residue dissolved in 500 ml. EtOAc, filtered, and the filtrate evaporated to dryness to yield Et 2-(2-diethylaminoethoxy)-4-nitrobenzoate (II); HCl salt, m. 144.4-5.2° (yield 45.5 g.). II with Sn and HCl gave the 4-amino analog (III); III.HCl, m. 134-5° (from Me2CO-EtOAc); III.2HCl, m. 173.6-3.9° (from absolute alc.-EtOAc); III.H3PO4, m. 168.7-9.6° (from 95% alc.). To 6 g. II in 50 ml. of EtOAc was added 15 ml. MeI, the solution refluxed 1.5 hrs., cooled, and the product filtered and washed with EtOAc; the II.MeI m. 143.1-4.6° (from iso-PrOH), was reduced by H and Pt at room temperature to III.MeI (IV) m. 139.2-41.1°. IV 10, PrCHO 5, PtO2 0.5 g. and 150 ml. absolute alc. treated at 50° with H under an unspecified pressure yielded Et 2-(2-diethylaminoethoxy)-4-(butylamino)benzoate-MeI. The following compds. having the general formula 3,4-RR1N(CH2)nO(R2O2C)C6H3NO2 are reported (n, R,R1,R2, salt, and m.p. of salt, resp., given): 2, Me, Me, Et, MeI, 190.2-1.2°; 2, Et, Et, Pr, HCl, 153.4-5.4° (MeI, 143.2-4.6°); 3, Et, Et, Et, HCl, 164.8-5.6° (MeI, 148-9.6°); 2, (NRR1 =) piperidino, Et, HCl 191-1.5° (MeI, 147.7-8.9°); 2, (NRR1 =) 2-methylpiperidino, Et, HCl 180.8-2.6° (MeI, 159.8-61.0°); 3, (NRR1 =) 2-methylpiperidino, Et, HCl, 158.2-9.6° (MeI

165.5-6.5°); 2, (NRR1 =) 2,6-dimethylpiperidino, Et, HCl
153-4° (MeI, 192.3-2.9°); 2, (NRR1 =) morpholino, Et, HCl,
207-8°. (MeI, m. 190.5-1.3°); 3, (NRR1 =) morpholino, Et,
HCl 142-4.6° (MeI, 161.1-1.7°); 2, Et, Et, Me, HCl,
156.9-9.2° (MeI, 162.5-3.0°); 2, (NRR1 =) morpholino, Me,
HCl, 206-6.4°, (MeI 209-11°). The following compds. having
the general formula 3,4-RR1N(CH2)nO(R2O2C)C6H3NH2 are reported: 2, Et, Et,
Me, MeI, m. 127.4-9.0°; 2, Et, Et, Pr, mono-H3PO4, 153-4°
(MeI m. 127.4-9.6°); 3, Et, Et, Et, H3PO4 151.5-3.2°, (MeI,
m. 125-6°); 2, (NRR1 =) piperidino, Et, H3PO4, 220.8-1.4°
(MeI, 167.4-8.4°; free base m. 107.3-8.5); 2, (NRR1 =)
2-methylpiperidino, Et, 91.2-2.4°; 2, (NRR1 =)
2,6-dimethylpiperidino, Et, H3PO4 211-11.8° (MeI
123.4-6.4°); 3, (NRR1 =) 2-methylpiperidino, Et, 112.4-3.5°
(H3PO4, 136.4-8.3°); 2, (NRR1 =) morpholino, Et, 98-9.8°
(H3PO4, 196.3-6.9°; MeI 182.7-3.7°); 3, (NRR1 =) morpholino,
Et, H3PO4, 143.4-4.4° (free base, m. 106.8-8.0°; MeI,
151.9-3.1°); 2, Me, Me, Et, H3PO4, 176.3-7.3° (MeI,
127.4-9.6°). Also reported is the preparation of Et
2-(2-chloroethoxy)-4-nitrobenzoate, m. 56.6-7.2°; Et
2-(2-diethylaminoethoxy)-4-(butylamino)benzoate-HCl, m. 160.5-1.8°.
All m. ps. are corrected

IT 878796-24-8, Ammonium, [2-(2-carboxy-5-nitrophenoxy)ethyl]diethylmethyl-, iodide (esters)

RN 878796-24-8 CAPLUS

CN Ethanaminium, 2-(2-carboxy-5-nitrophenoxy)-N,N-diethyl-N-methyl-, iodide (1:1) (CA INDEX NAME)



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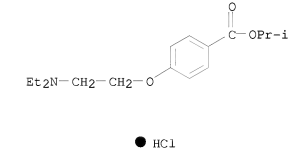
L4 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1938:41768 CAPLUS
DOCUMENT NUMBER: 32:41768
ORIGINAL REFERENCE NO.: 32:5807a-c
TITLE: Amino ethers of phenolic benzoic esters
AUTHOR(S): Rohmann, C.; Koch, A.
SOURCE: Archiv der Pharmazie und Berichte der Deutschen Pharmazeutischen Gesellschaft (1938), 276, 154-64
CODEN: APBDAJ; ISSN: 0376-0367
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
AB cf. C. A. 30, 4160.7. In the present study the carboxy group of p-HOC6H4CO2H has been esterified with different alcs., while the HO group was etherified with Et2NCH2CH2OH. The alkaline ethers thus carry a tertiary N radical. This ever-present group stands in the p-position to a varying ester group. This arrangement conditions the local anesthetic action. With the aid of the organoleptic test, it was found that all the compds. prepared were more or less locally anesthetic. The change in activity, since the ether group remained constant, must therefore depend on the variation of the alkyl radical in the ester group. All the compds. were tested along with novocaine, tutocaine, cocaine and pantocaine with respect to their physicochem. properties, and the results obtained herein reported. Among the alkyl p-diethylaminoethoxybenzoate-HCl prepared were: Et, m. 154°; Pr, m. 103°; iso-Pr m. 146°; Bu m. 74°; iso-Bu m. 92°; allyl, m. 176-7°.
IT 1071582-57-4P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Amino ethers of phenolic benzoic esters)
RN 1071582-57-4 CAPLUS
CN Benzoic acid, 4-[2-(diethylamino)ethoxy]-, 1-methylethyl ester, hydrochloride (1:1) (CA INDEX NAME)



L4 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1934:60903 CAPLUS
DOCUMENT NUMBER: 28:60903
ORIGINAL REFERENCE NO.: 28:7429h-i,7430a-b
TITLE: Dialkylaminoalkyl esters of hydroxy-3-carboxybiphenyls
INVENTOR(S): Christiansen, Walter G.; Harvey, Adelbert W.
PATENT ASSIGNEE(S): E. R. Squibb & Sons
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 1976922		19341016	US	<--

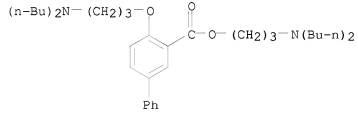
AB Compds. (suitable for use as local anesthetics in solution buffered with a phosphate) such as the dialkylaminoalkyl esters of 3 - carboxy - 4 - hydroxybiphenyl and 3 - carboxy - 2-hydroxybiphenyl and salts thereof, particularly 3-β-diethylaminocarbethoxy-4-hydroxybiphenyl and its

salts are prepared by converting the hydroxy-3-carboxybiphenyl to a salt, forming a halide ester, preferably a bromoalkyl ester from the salt and then forming the dialkylaminoalkyl ester from this. Purification of the 3-β-diethylaminocarbethoxy-4-hydroxybiphenyl hydrochloride may be accomplished by crystallization from absolute EtOH. The product, in the form of the hydrochloride, is a white crystalline substance soluble in water, m. 167-168.5°. The free ester is an almost colorless oil. Starting with 3-carboxy-2-hydroxybiphenyl and employing similar reactions, corresponding alkyl derivs. may be formed in which the hydroxy group is in the 2- instead of the 4-position.

IT 873986-35-7, Benzoic acid, 2-(γ-dibutylaminopropoxy)-5-phenyl-, γ-dibutylaminopropyl ester
(and salts)

RN 873986-35-7 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 4-[3-(dibutylamino)propoxy]-, 3-(dibutylamino)propyl ester (CA INDEX NAME)



L4 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1934:60902 CAPLUS

DOCUMENT NUMBER: 28:60902

ORIGINAL REFERENCE NO.: 28:7429g-h

TITLE: Dialkylaminoalkyl esters of dialkylaminoalkoxy-3-carboxybiphenyl

INVENTOR(S): Christiansen, Walter G.; Braker, William

PATENT ASSIGNEE(S): E. R. Squibb & Sons

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 1976921		19341016	US	<--

AB Compds. (suitable for use in the preparation of local anesthetics) such as 3-β-diethylaminocarbethoxy-4-β-diethylaminoethoxybiphenyl and 3-γ-dibutylaminocarbopropoxy - 4 - γ - dibutylaminopropoxybiphenyl are prepared from a hydroxy-3-carboxybiphenyl by forming its di-Na derivative and then replacing the Na atoms by dialkylaminoalkyl radicals (various details for preparing these compds. and their hydrochlorides and borates being given).

IT 873986-35-7, Benzoic acid, 2-(γ-dibutylaminopropoxy)-5-phenyl-, γ-dibutylaminopropyl

ester
(and salts)
RN 873986-35-7 CAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid, 4-[3-(dibutylamino)propoxy]-, 3-(dibutylamino)propyl ester (CA INDEX NAME)